

PORTLAND HARBOR SUPERFUND SITE
BIOACCUMULATION MODELING REPORT

**APPENDIX B: MECHANISTIC MODEL
PARAMETERIZATION**

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LIST OF ACRONYMS

Acronym	Definition
ATSDR	Agency for Toxic Substances and Disease Registry
BCF	bioconcentration factor
BERA	baseline ecological risk assessment
BIC	benthic invertebrate consumer
BIF	benthic invertebrate filter feeder
<u>BSAF</u>	<u>biota-sediment accumulation factor</u>
<u>EIC</u>	<u>epibenthic invertebrate consumer</u>
<u>CARP</u>	<u>Contaminant Assessment and Reduction Project</u>
<u>CDD</u>	<u>chlorodibenzo-<i>p</i>-dioxin</u>
<u>CDF</u>	<u>chlorodibenzofuran</u>
cfs	cubic feet per second
DBP	dichlorobenzophenone
DDD	dichlorodiphenyldichloroethane
DDE	dichlorodiphenyldichloroethylene
DDT	dichlorodiphenyltrichloroethane
DF	detection frequency
<u>DL</u>	<u>detection limit</u>
DOC	dissolved organic carbon
EDA	dietary chemical transfer constant A
EDB	dietary chemical transfer constant B
EDI	equal depth integrated
<u>EIC</u>	<u>epibenthic invertebrate consumer</u>
EPA	US Environmental Protection Agency
ESB	equilibrium sediment partitioning benchmark
FPW	fraction of porewater ventilated
K _M	metabolic rate constant
K _T	total elimination rate
K _{OW}	octanol-water partition coefficient
LASAR	Laboratory Analytical Storage and Retrieval
<u>LWR</u>	<u>Lower Willamette River</u>
NB	near bottom
NLOC	non-lipid organic carbon
NLOM	non-lipid organic matter
NS	near surface
ODEQ	Oregon Department of Environmental Quality

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Acronym	Definition
ODFW	Oregon Department of Fish and Wildlife
PCB	polychlorinated biphenyl
PRG	preliminary remediation goal
RAIS	risk assessment information system
RI/FS	risk investigation/feasibility study
RM	river mile
SPARC	SPARC Performs Automated Reasoning in Chemistry
SWAC	spatially weighted average concentration
TOC	total organic carbon
total DDx	sum of all six DDT isomers (2,4'-DDD, 2,4'-DDE, 2,4'-DDT, 4,4'-DDD, 4,4'-DDE and 4,4'-DDT)
TSS	total suspended solids
UA	uptake constant A
UB	uptake constant B
VI	vertically integrated
XAD	Infiltrex™ system with XAD resin column

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1.0 SUMMARY OF APPROACH TO PARAMETER VALUES AND DISTRIBUTIONS

The input parameters required by the adaptation of the Arnot and Gobas bioaccumulation model (Arnot and Gobas 2004) used in this report were derived from site-specific data whenever possible. The main sources of site-specific data were the Round 1 through Round 3 data collected and analyzed for the Portland Harbor remedial investigation/feasibility study (RI/FS). Literature values were used when an input parameter could not be defined using these data.

In order to reflect the uncertainty regarding the values of parameters based on site-specific or literature-derived information, statistical distributions were defined for most parameters. Once distributions had been assigned to the input parameters, the model could be run either probabilistically, using distributions, or deterministically, using point estimates for parameter values. The results of probabilistic model runs were distributions for predicted tissue concentrations (i.e., model output) based on random selection of input parameter values from the defined input distributions. Because the focus of the model was on prediction of average tissue concentrations, the input parameter distributions were intended to bound uncertainty on estimates of the central tendency of parameter values. Parameter values from within these distributions were selected for the calibrated version of the model and used in the development of preliminary remediation goals (PRGs). This attachment discusses the parameter distributions in detail and the sources used to develop each distribution.

2.0 RULES FOR ASSIGNING DISTRIBUTIONS

For input into the model, parameter distributions were defined based on shape (e.g., uniform distribution) and descriptive statistics (e.g., mean and standard error or nominal value, maximum, and minimum). The selected distributions were based on empirical data whenever possible and were intended to reflect the uncertainty surrounding estimates of central tendency. Based on the central limit theorem, the distribution of estimates of the mean approaches a normal distribution with sufficient sample size, and the standard deviation of the distribution of estimates of the mean is defined by the standard error of the original data. The following standardized approach was used to develop parameter estimates for the distributions of central tendency.

1. When site-specific data were available, estimates of the mean were defined by a normal distribution with a mean equal to the mean of the empirical data and a standard deviation equal to the standard error of the empirical data.
2. If there were no site-specific data, but literature values for the mean and standard deviation were available, the literature mean and standard deviation were used to define a normal distribution that would provide a conservative bounding of the distribution of mean estimates.
3. For all chemicals or chemical groups modeled, a uniform distribution was assigned for the log of the octanol-water partition coefficient (log K_{OW} , hereafter referred to as the K_{OW}) for a given chemical group. The nominal value was defined as the most appropriate K_{OW} based on the literature reviewed and in consideration of site-specific data for chemical mixtures (e.g., for total polychlorinated biphenyls [PCBs], the concentrations of different PCB congeners in tissue were considered to account for the differing contributions of the individual congeners to the total). The range was defined as minimum to maximum literature K_{OW} values.
4. For all other parameters with insufficient data to define a distribution (i.e., mean and standard deviation or standard error), a triangle or uniform distribution was assigned (MacIntosh et al. 1994). The nominal value was defined as the mean of the data if the data were considered sufficiently relevant and comprehensive. For more uncertain data, the nominal value was based on the consideration of published selections for parameter values used in other mechanistic models (Gobas and Arnot 2005; Arnot and Gobas 2004) and best professional judgment. The minimum and maximum values were defined by the literature values if they were considered sufficient to bound a plausible range.

Based on comments from the US Environmental Protection Agency (EPA) on the mechanistic model developed as part of the Round 2 Report, 21 parameters calibrated as part of the Round 2 Report mechanistic model were not calibrated for this version of the mechanistic model (EPA 2008a). These parameters include uptake constant A and B (Section 5.1), the non-lipid organic matter (NLOM)-proportionality constant (Section 5.3),

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and the species-specific dietary absorption efficiencies of lipid organic matter and NLOM
(Section 6.2).

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3.0 CHEMICAL DATA

Two chemical-specific parameters are required for the adaptation of the Arnot and Gobas model used in this report: the K_{OW} and the Henry's Law constant. Because the Henry's Law constant cancels itself out in the model calculations, no values were entered for this parameter. Thus, the only chemical-specific parameter required for this model was the K_{OW} . The same K_{OW} value is used throughout the model, regardless of medium.

For each chemical modeled, a literature search was conducted from the following sources to compile possible K_{OW} values:

- EPA guidance documents for developing equilibrium sediment partitioning benchmarks (ESBs) (EPA 2008c)
- SPARC (SPARC Performs Automated Reasoning in Chemistry) online database (University of Georgia 2007)
- *Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals* (Mackay et al. 2006)
- Oak Ridge National Laboratory – Risk Assessment Information System (RAIS) (RAIS 2008)
- Agency for Toxic Substances and Disease Registry (ATSDR) ToxFAQs (ATSDR 2008)
- EPA's KowWIN software (EPA 2007)

For those chemicals that were modeled individually (e.g., PCB 126 and 4,4'-dichlorodiphenyltrichloroethane [DDT]), the best-estimate literature value was selected from EPA's ESB guidance documents when available, or from the SPARC database. A uniform distribution was used for the K_{OW} when calibrating the mechanistic model, with the distribution range equal to the minimum and maximum values from the above literature sources. Table 3-1 shows the individual chemicals and the K_{OW} values to be used in the mechanistic model.

Table 3-1. K_{OW} Values for Individual Chemicals Used in the Mechanistic Model

Analyte	Literature log K_{OW} Values		
	Primary	Minimum	Maximum
PCBs			
PCB 17	5.70	4.60	5.76
PCB 77	6.22	5.62	7.87
PCB 118	6.85	6.24	7.42
PCB 126	6.83	6.38	7.00

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Table 3-1. K_{ow} Values for Individual Chemicals Used in the Mechanistic Model

Analyte	Literature log K _{ow} Values		
	Primary	Minimum	Maximum
PCB 167	7.48	6.82	7.62
Dioxins and Furans			
2,3,4,7,8-PeCDF	6.95	6.56	7.82
Pesticides			
4,4'-DDD	6.05	4.82	6.33
4,4'-DDE	6.90	4.28	6.97
4,4'-DDT	6.72	3.98	8.31
Aldrin	6.39	3.01	7.50
alpha-HCH	3.78	3.19	4.57
beta-HCH	3.78	3.19	4.26
Dieldrin	5.37	2.60	6.20
gamma-HCH	3.73	3.19	4.26
Heptachlor	6.03	3.87	6.10
Heptachlor epoxide	5.29	3.65	5.42
Total chlordane	6.42	2.78	6.42

DDD – dichlorodiphenyldichloroethane
DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
HCH – hexachlorocyclohexane
K_{ow} – octanol-water partition coefficient
PCB – polychlorinated biphenyl
~~PeCDF – pentachlorodibenzofuran~~

For the modeled chemical mixtures (i.e., total PCBs, sum dichlorodiphenyldichloroethane [DDD], sum dichlorodiphenyldichloroethylene [DDE], sum DDT, and total DDx), K_{ow} values were weighted based on the percent contribution of the individual components to account for the differing contributions of the individual congeners to the total. Literature values for the individual components were developed as described above in Section 3.0, and were then weighted based on the average percent contribution across tissue samples for which the components were measured to best represent the mixture of PCBs that is present in the ~~LWR~~ Lower Willamette River (i.e., all Portland Harbor Study Area fish and invertebrate tissue samples with the exception of laboratory-exposed clams, laboratory-exposed worms, and multiplate invertebrates). Primary values and distributions were developed using the same process described above, except that the weighted K_{ow} values were used. Table 3-2 shows the chemical mixtures and the K_{ow} values to be used in the model.

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Table 3-2. Kow Values for Chemical Mixtures

Chemical	Literature log Kow Values		
	Primary	Minimum	Maximum
PCBs			
Total PCBs ^a	7.40	6.09	7.84
Pesticides			
Sum DDD	6.00	4.80	6.31
Sum DDE	6.80	4.22	6.87
Sum DDT	6.58	3.98	8.19
Total DDx	6.65	4.34	7.08

^a The total PCB Kow values are based only on PCB congeners.

DDD – dichlorodiphenyldichloroethane

DDE – dichlorodiphenyldichloroethylene

DDT – dichlorodiphenyltrichloroethane

Kow – octanol-water partition coefficient

PCB – polychlorinated biphenyl

total DDx – sum of all six DDT isomers (2,4'-DDD, 2,4'-DDE, 2,4'-DDT, 4,4'-DDD, 4,4'-DDE, and 4,4'-DDT)

Literature values for individual chemical constituents, along with their average percent contribution based on fish and invertebrate tissue are shown in Table 3-3.

Table 3-3. Kow Values for Components of Calculated Chemical Mixtures

Chemical	Average Contribution (fraction) ^a	Log Kow		
		Primary	Minimum	Maximum
Total PCBs				
PCB 001	0.00142	4.61	3.75	4.80
PCB 002	0.0000205	4.55	3.75	4.81
PCB 003	0.000129	4.56	4.26	4.90
PCB 004	0.00391	5.13	3.02	5.70
PCB 005	0.0000184	5.22	4.82	5.22
PCB 006	0.000327	5.07	4.84	5.07
PCB 007	0.0000343	5.15	4.67	5.30
PCB 008	0.00124	5.07	4.47	5.51
PCB 009	0.0000591	5.14	4.67	5.30
PCB 010	0.000104	5.23	4.93	5.31
PCB 011	0.00179	5.01	5.01	5.4
PCB 012 & 013	0.0000858	5.09	5.05	5.51
PCB 014	0.0000117	5.11	5.05	5.63
PCB 015	0.000618	5.02	4.82	5.58
PCB 016	0.00137	5.75	4.15	5.75
PCB 017	0.00287	5.70	4.60	5.76

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Table 3-3. Kow Values for Components of Calculated Chemical Mixtures

Chemical	Average Contribution (fraction) ^a	Log Kow		
		Primary	Minimum	Maximum
PCB 018 & 030	0.0036	5.76	3.89	6.22
PCB 019	0.00267	5.74	3.75	5.74
PCB 020 & 028	0.00969	5.66	4.69	5.75
PCB 021 & 033	0.00235	5.75	5.48	5.98
PCB 022	0.00225	5.69	4.84	5.69
PCB 023	0.0000134	5.81	5.44	5.81
PCB 024	0.0000389	5.84	4.52	5.84
PCB 025	0.000613	5.62	5.51	5.69
PCB 026 & 029	0.00134	5.69	5.51	6.25
PCB 027	0.000927	5.70	5.24	5.70
PCB 031	0.00513	5.61	5.30	6.33
PCB 032	0.00151	5.70	4.60	5.80
PCB 034	0.0000406	5.63	5.51	5.71
PCB 035	0.0000579	5.61	5.53	5.82
PCB 036	0.000042	5.57	4.15	5.88
PCB 037	0.00147	5.62	4.94	6.00
PCB 038	0.0000166	5.78	5.48	5.78
PCB 039	0.0000744	5.58	5.58	5.89
PCB 040 & 041 & 071	0.00615	6.35	4.63	6.35
PCB 042	0.00407	6.31	5.72	6.34
PCB 043	0.000512	6.34	5.75	6.34
PCB 044 & 047 & 065	0.0223	6.34	4.79	7.87
PCB 045 & 051	0.00309	6.32	4.84	6.34
PCB 046	0.000379	6.36	4.84	6.36
PCB 048	0.00236	6.32	5.56	6.34
PCB 049 & 069	0.0125	6.28	5.73	6.41
PCB 050 & 053	0.00384	6.32	5.39	7.87
PCB 052	0.0199	6.20	3.91	6.34
PCB 054	0.0005	6.34	4.16	7.13
PCB 055	0.0001	6.31	5.86	6.34
PCB 056	0.00374	6.29	5.85	6.34
PCB 057	0.0000824	6.28	5.91	6.34
PCB 058	0.0000701	6.25	5.91	6.34
PCB 059 & 062 & 075	0.00149	6.37	5.79	6.37
PCB 060	0.00391	6.31	5.33	7.87
PCB 061 & 070 & 074 & 076	0.0246	6.31	5.86	6.79
PCB 063	0.000996	6.28	5.91	6.34

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Table 3-3. Kow Values for Components of Calculated Chemical Mixtures

Chemical	Average Contribution (fraction) ^a	Log Kow		
		Primary	Minimum	Maximum
PCB 064	0.00631	6.30	5.76	6.34
PCB 066	0.0197	6.23	5.8	6.34
PCB 067	0.000361	6.24	5.93	6.4
PCB 068	0.000259	6.17	5.99	6.34
PCB 072	0.000271	6.16	5.98	7.87
PCB 073	0.000136	6.26	5.80	6.34
PCB 077	0.00102	6.22	5.62	7.87
PCB 078	0.0000179	6.23	5.95	6.35
PCB 079	0.000314	6.18	6.00	6.42
PCB 080	0.0000198	6.13	6.13	6.85
PCB 081	0.0000442	6.23	5.96	6.64
PCB 082	0.0017	7.00	6.05	7.00
PCB 083 & 099	0.0276	6.92	6.05	7.21
PCB 084	0.00364	6.95	5.60	6.98
PCB 085 & 116 & 117	0.00692	7.04	6.23	7.04
PCB 086 & 087 & 097 & 108 & 119 & 125	0.0174	6.93	5.45	8.71
PCB 088 & 091	0.0046	6.95	5.87	7.51
PCB 089	0.000179	6.99	5.6	6.99
PCB 090 & 101 & 113	0.0372	6.87	5.58	6.98
PCB 092	0.00773	6.88	6.05	6.98
PCB 093 & 095 & 098 & 100 & 102	0.0244	6.94	5.18	6.98
PCB 094	0.000339	6.95	6.04	6.98
PCB 096	0.000257	6.94	5.54	6.98
PCB 103	0.000867	6.89	5.92	8.71
PCB 104	0.0000973	6.96	5.37	8.71
PCB 105	0.013	6.91	4.97	7.14
PCB 106	0.0000253	6.95	6.29	7.22
PCB 107 & 124	0.000866	6.85	6.35	6.98
PCB 109	0.00332	6.96	6.27	6.98
PCB 110 & 115	0.0284	6.94	6.20	6.98
PCB 111	0.00008	6.84	6.39	8.27
PCB 112	0.0000547	6.94	6.24	6.98
PCB 114	0.00102	6.95	6.29	6.98
PCB 118	0.04	6.85	6.24	7.42
PCB 120	0.0003	6.80	5.22	6.98
PCB 121	0.0000895	6.88	6.19	6.98
PCB 122	0.000218	6.90	6.29	6.98

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Table 3-3. Kow Values for Components of Calculated Chemical Mixtures

Chemical	Average Contribution (fraction) ^a	Log Kow		
		Primary	Minimum	Maximum
PCB 123	0.000737	6.83	6.19	6.98
PCB 126	0.0000788	6.83	6.38	7.00
PCB 127	0.000137	6.79	6.42	6.98
PCB 128 & 166	0.00722	7.58	6.40	7.62
PCB 129 & 138 & 160 & 163	0.083	7.58	6.39	7.90
PCB 130	0.00346	7.60	6.57	7.62
PCB 131	0.000348	7.63	6.38	7.63
PCB 132	0.0104	7.58	6.20	7.62
PCB 133	0.00186	7.56	6.60	7.69
PCB 134 & 143	0.00194	7.62	6.20	7.62
PCB 135 & 151 & 154	0.0236	7.54	5.94	7.62
PCB 136	0.00481	7.54	4.91	8.35
PCB 137	0.00277	7.58	6.71	7.71
PCB 139 & 140	0.000977	7.59	6.49	7.62
PCB 141	0.00962	7.56	6.64	9.54
PCB 142	0.0000205	7.73	6.41	7.73
PCB 144	0.00241	7.54	6.29	7.62
PCB 145	0.0000126	7.61	6.25	7.62
PCB 146	0.018	7.53	6.57	7.62
PCB 147 & 149	0.0411	7.53	6.14	7.62
PCB 148	0.000305	7.55	5.74	7.62
PCB 150	0.000193	7.54	6.16	7.62
PCB 152	0.000101	7.58	6.09	7.62
PCB 153 & 168	0.114	7.53	6.34	8.35
PCB 155	0.0000508	7.57	6.01	7.62
PCB 156	0.00737	7.56	6.70	7.84
PCB 156 & 157	0.0068	7.55	6.70	7.84
PCB 157	0.00108	7.54	6.73	7.62
PCB 158	0.00646	7.57	6.69	7.69
PCB 159	0.00045	7.51	6.76	7.62
PCB 161	0.00000809	7.53	6.66	7.62
PCB 162	0.000226	7.51	6.66	7.62
PCB 164	0.00334	7.53	6.63	7.62
PCB 165	0.000109	7.50	6.57	7.62
PCB 167	0.00321	7.48	6.82	7.62
PCB 169	0.0000237	7.46	7.01	7.62
PCB 170	0.0197	8.28	6.83	8.28

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Table 3-3. Kow Values for Components of Calculated Chemical Mixtures

Chemical	Average Contribution (fraction) ^a	Log Kow		
		Primary	Minimum	Maximum
PCB 171 & 173	0.00617	8.31	6.68	8.31
PCB 172	0.00375	8.24	6.85	8.27
PCB 174	0.0103	8.23	6.85	8.27
PCB 175	0.00091	8.22	6.92	8.27
PCB 176	0.0017	8.22	6.55	8.27
PCB 177	0.0115	8.23	6.73	8.27
PCB 178	0.00593	8.19	6.85	8.27
PCB 179	0.00649	8.19	6.41	8.27
PCB 180 & 193	0.0677	8.20	6.56	8.27
PCB 181	0.000229	8.29	7.06	8.29
PCB 182	0.000132	8.23	6.92	8.27
PCB 183 & 185	0.0179	8.24	6.78	8.27
PCB 184	0.0000386	8.21	6.65	8.27
PCB 186	0.00000937	8.34	6.69	8.34
PCB 187	0.0436	8.17	6.76	8.27
PCB 188	0.0000912	8.19	6.78	8.27
PCB 189	0.000808	8.18	6.75	8.27
PCB 190	0.005	8.30	7.05	8.3
PCB 191	0.00107	8.20	7.12	8.27
PCB 192	0	8.25	7.09	8.27
PCB 194	0.00861	8.91	6.94	9.35
PCB 195	0.00399	8.98	6.95	8.98
PCB 196	0.00515	8.90	7.42	8.91
PCB 197 & 200	0.00102	8.91	7.16	8.91
PCB 198 & 199	0.0099	8.91	7.20	8.91
PCB 201	0.00138	8.86	7.21	8.91
PCB 202	0.00252	8.83	6.98	9.77
PCB 203	0.00678	8.92	6.93	8.92
PCB 204	0.0000203	8.94	7.26	8.94
PCB 205	0.000442	8.93	7.47	8.93
PCB 206	0.00228	9.62	7.07	9.62
PCB 207	0.000407	9.61	7.52	9.61
PCB 208	0.000812	9.58	7.69	9.58
PCB 209	0.00102	10.3	7.59	11.2
Sum DDD				
2,4'-DDD	0.224	5.93	4.82	6.33
4,4'-DDD	0.772	6.05	4.82	6.33

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Table 3-3. Kow Values for Components of Calculated Chemical Mixtures

Chemical	Average Contribution (fraction) ^a	Log K _{ow}		
		Primary	Minimum	Maximum
Sum DDE				
2,4'-DDE	0.0428	6.84	4.28	6.97
4,4'-DDE	0.943	6.90	4.28	6.97
Sum DDT				
2,4'-DDT	0.318	6.57	3.98	8.31
4,4'-DDT	0.668	6.72	3.98	8.31
Total DDx				
2,4'-DDD	0.0501	5.93	4.82	6.33
2,4'-DDE	0.0202	6.84	4.28	6.97
2,4'-DDT	0.0671	6.57	3.98	8.31
4,4'-DDD	0.183	6.05	4.82	6.33
4,4'-DDE	0.549	6.90	4.28	6.97
4,4'-DDT	0.13	6.72	3.98	8.31

^a All Portland Harbor Study Area fish and invertebrate tissue samples (with the exception of laboratory-exposed clams, laboratory-exposed worms, and multiplate invertebrates) were used to calculate the average percent contribution of each chemical.

DDD – dichlorodiphenyldichloroethane

DDE – dichlorodiphenyldichloroethylene

DDT – dichlorodiphenyltrichloroethane

K_{ow} – octanol-water partition coefficient

PCB – polychlorinated biphenyl

total DDx – sum of all six DDT isomers (2,4'-DDD, 2,4'-DDE, 2,4'-DDT, 4,4'-DDD, 4,4'-DDE, and 4,4'-DDT)

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4.0 ENVIRONMENTAL DATA

The environmental input parameters needed for the Arnot and Gobas model used in this report are based on the surface water and sediment data for the Lower Willamette River (~~LWR~~). All parameters were calculated using site-specific data from the project database or the Oregon Department of Environmental Quality (ODEQ) Web site (ODEQ 2008).

4.1 WATER DATA

The water input parameters required for the Arnot and Gobas model are temperature, total suspended solids (TSS), dissolved organic carbon (DOC), and dissolved chemical concentrations in the water column. Particulate organic carbon (POC) is not included in the FWM because dissolved water concentrations were available from the ~~LWR~~Lower Willamette River, thus removing one area of uncertainty from model calculations.

Water sample locations in the ~~LWR~~Lower Willamette River are shown on Map 4-1.

4.1.1 Temperature Data

Sampling events for the Portland Harbor RI/FS at the conclusion of Round 2 were limited to seven events over 2.5 years. Therefore, water temperature data for the site were taken from the Laboratory Analytical Storage and Retrieval (LASAR) database provided online by ODEQ (2008). A map of the river on the ODEQ Web site was used to choose stations that were located within the Study Area (River Mile [RM] 2 to RM 11). Thirteen stations were identified, but water temperature data were available for only seven of these stations from January 11, 1995 through April 14, 2008 (n = 4,248). These seven stations are listed below, along with their station identification numbers from the LASAR database and their approximate location:

- Willamette River upstream of Oregon Steel Mills, City of Portland site (No. 29746) – between RM 2 and RM 3
- Willamette River at US Government moorings (No. 30755) – RM 6
- Willamette River at St. John's Bridge (No. 10821) – RM 6
- Willamette River at SP&S RR Bridge, Portland (No. 10332) – RM 7
- Willamette River at St. John's RR Bridge, City of Portland site (No. 28765) – between RM 7 and RM 8
- Swan Island Channel Midpoint (No. 10801) – RM 8.5 in the Swan Island Lagoon
- Swan Island Channel Boat Ramp (No. 10802) – RM 9 in the Swan Island Lagoon

The number of samples taken per year per location was variable during the period from January 11, 1995 to April 14, 2008. An average was calculated for each month across all

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years between 1995 and 2008 (e.g., mean January temperature included all samples collected at all locations for all years during the month of January). The 12 monthly averages were used to calculate a yearly average. The mean temperature was 13.9°C, with a standard error of 1.7°C over a 12-month period. To describe uncertainty about this estimate of the mean, a normal distribution was assigned with a standard deviation of the distribution equal to the standard error of the data.

4.1.2 Water Chemistry Data

Chemical concentrations in the water column for use in the mechanistic model were calculated using XAD water column samples collected during the seven sampling events at the five transect locations, as summarized in Section 5.3.5.2.1 of the Bioaccumulation Modeling Report and further discussed here. Table 4-1 provides a summary of the sampling events and locations used to calculate the Study Area-wide water averages.

Table 4-1. Summary of Surface Water Sampling Events

Sampling Event Information			Sampling Locations				
Date	Season	Flow Condition ^a	W027 (Multnomah Channel)	W025 (RM 2)	W005 (RM 3.9)	W011 (RM 6.3)	W023 (RM 11)
Round 2a							
November 2004	Fall	Low flow			EDI	EDI	EDI
March 2005	Winter	Low flow			EDI	EDI	EDI
July 2005	Summer	Low flow			EDI	EDI	EDI
Round 3a							
January 2006	Winter	High flow			NB/NS		VI
September 2006	Summer	Low flow	NB/NS	VI	NB/NS	NB/NS	VI
November 2006	Fall	Stormwater	NB/NS	VI	NB/NS	NB/NS	VI
January – March 2007	Winter	High flow	NB/NS	VI	NB/NS	NB/NS	VI

^a Low-flow conditions were rates less than 50,000 cfs, while high-flow conditions were flow rates above this level.
cfs – cubic feet per second

EDI – equal depth integrated (1 sample per event)

NB/NS – near bottom/near surface (2 samples per event)

VI – vertically integrated (3 samples per event, taken at east, middle, and west points across river)

The following steps were taken to calculate a Study Area-wide average chemical concentration in water:

1. **Event-location averages:** Calculate an average for each event-location pair when necessary (i.e., the near-bottom and near-surface samples were averaged together and the east, middle, and west samples were averaged together).

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2. **Event averages:** Calculate the average across the locations to generate an average for each event.
3. **Low flow and high flow averages:** Calculate a low-flow average and a high-flow average. Note that the stormwater event (November 2006) was included in the low-flow average because it was a low-flow stormwater event.
4. **Study Area-wide average:** Calculate the overall average concentration using the weighting values. Based on the temporal (daily count) average of the hydrographs, the high-flow average was weighted as 22% of the total; while the low-flow/stormwater average was weighted as 78% of the total (Portland Harbor RI/FS draft final remedial investigation report (Integral et al. 2011)).

In the process described above, only detected values were included in the averaging. If there were no detected values, one-half of the maximum reporting limit was used.

Uncertainty in the Study Area-wide chemical concentrations in surface water was introduced by two elements:

- Averaging of chemical concentrations under high-flow and low-flow conditions
- Weighting of values based on the count days meeting high-flow and low-flow conditions

The standard errors for the high-flow and low-flow events were calculated, and then weighted using the same weighting values applied when calculating the Study Area-wide average concentrations. Because of the high level of uncertainty in the high-flow and low-flow averages, the uncertainty in the weighting values was not considered when calculating the distribution to be used during model calibration. The standard error used for distribution in the model was equal to the standard errors from the high- and low-flow events weighted in the same way as the mean surface water concentration. Table 4-2 shows the average and standard error surface water concentrations for the high-flow and low-flow values, along with the values used in the model to define the normal distribution.

Table 4-2. Chemical Concentrations in Surface Water

Analyte	DF	Surface Water Concentrations (ng/L)					
		High Flow		Low Flow		Model Values ^a	
		Mean	SE	Mean	SE	Mean	SE
PCBs							
PCB 17	26/26	0.00135	0.000131	0.00518	0.000719	0.00434	0.000590
PCB 77	24/26	9.99×10 ⁻⁵	6.28×10 ⁻⁶	0.000307	4.82×10 ⁻⁵	2.61×10 ⁻⁴	3.90×10 ⁻⁵
PCB 118	26/26	0.00125	0.000114	0.00326	0.000287	0.00282	0.000249
PCB 126	5/26	ND ^b	ND ^b	1.32×10 ⁻⁵	1.04×10 ⁻⁶	1.32×10 ⁻⁵	1.04×10 ⁻⁶
PCB 167	22/26	5.48×10 ⁻⁵	7.42×10 ⁻⁶	1.13×10 ⁻⁴	8.44×10 ⁻⁶	1.00×10 ⁻⁴	8.22×10 ⁻⁶
Total PCBs ^c	26/26	0.0746	0.00585	0.257	0.0296	0.217	0.0244

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Table 4-2. Chemical Concentrations in Surface Water

Analyte	DF	Surface Water Concentrations (ng/L)					
		High Flow		Low Flow		Model Values ^a	
		Mean	SE	Mean	SE	Mean	SE
Dioxins and Furans							
2,3,4,7,8-PeCDF	7/26	3.33×10 ⁻⁶	5.77×10 ⁻⁷	5.71×10 ⁻⁶	6.02×10 ⁻⁷	5.19×10 ⁻⁶	5.97×10 ⁻⁷
Pesticides							
4,4'-DDD	26/26	0.023	0.002	0.056	0.011	0.049	0.0090
4,4'-DDE	26/26	0.054	0.0035	0.024	0.0026	0.031	0.0028
4,4'-DDT	26/26	0.056	0.0075	0.0058	0.00057	0.017	0.0021
Aldrin	23/26	0.0022	0.00014	0.0022	0.00024	0.0022	0.00022
alpha-HCH	26/26	0.02	0.0024	0.029	0.0045	0.027	0.0040
beta-HCH	20/26	0.0032	0.00019	0.0057	0.00049	0.0052	0.00042
Dieldrin	26/26	0.18	0.036	0.035	0.0017	0.067	0.0092
gamma-HCH	26/26	0.016	0.0013	0.027	0.0013	0.025	0.0013
Heptachlor	3/26	ND ^b	ND ^b	0.00021	0.000016	0.00021	0.000016
Heptachlor epoxide	26/26	0.0175	0.00141	0.0042	0.00017	0.0071	0.00044
Sum DDD	26/26	0.031	0.0033	0.081	0.016	0.070	0.013
Sum DDE	26/26	0.055	0.0034	0.025	0.0028	0.032	0.0029
Sum DDT	26/26	0.068	0.0081	0.0084	0.00085	0.022	0.0024
Total chlordane	26/26	0.042	0.0028	0.025	0.0017	0.029	0.0019
Total DDx	26/26	0.15	0.011	0.12	0.019	0.13	0.017

Note: When calculating mean and SE values, only detected values were used in the calculations.

^a The standard error of the data was used to describe the standard deviation of estimates of the mean.

^b Because there was no data for the high flow events, the low flow concentrations were used in the model.

^c Sum of PCB congeners.

DDD – dichlorodiphenyldichloroethane

DDE – dichlorodiphenyldichloroethylene

DDT – dichlorodiphenyltrichloroethane

DF – detection frequency

HCH – hexachlorocyclohexane

ND – no detected data

PCB – polychlorinated biphenyl

SE – standard error

total DDx – sum of all six DDT isomers (2,4'-DDD, 2,4'-DDE, 2,4'-DDT, 4,4'-DDD, 4,4'-DDE, and 4,4'-DDT)

4.1.3 Total Suspended Solids Data

The concentration of TSS was calculated using data collected for the Portland Harbor RI/FS. Because the TSS parameter affects only the feeding rate for benthic invertebrate filter feeders (clams), it was determined that TSS data from near-bottom samples would be the most appropriate. Each of the 32 near-bottom sample locations in the Study Area was sampled at least once during the seven surface water sampling events that were described in Table 4-1. TSS concentrations for use in the mechanistic model were calculated using the same

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methodology as described above for water chemistry data (Section 4.1.2). The mean TSS value calculated for this model was 1.13×10^{-5} kg/L, and a normal distribution with a standard deviation of 4.5×10^{-6} kg/L (defined by the weighted standard error of the empirical data as was done for the chemical concentration in water data) was used to for the model distribution.

4.1.4 Dissolved Organic Carbon Data

The average DOC value used in the mechanistic model was calculated using XAD water column samples collected during the seven sampling events at the five transect locations. DOC concentrations for use in the model were calculated using the same methodology as described above for water chemistry data (Section 4.1.2). A normal distribution was used to define the DOC parameter distribution, with a mean value of 1.38×10^{-6} kg/L and a standard deviation of 5.9×10^{-8} kg/L (defined by the weighted standard error of the empirical data as was done for the chemical concentration in water data).

4.2 SEDIMENT DATA

The sediment input parameters required for the Arnot and Gobas model include the total organic carbon (TOC) concentration and the chemical concentration in the sediment. In order to reduce spatial bias in the available sediment chemistry data for the site, a spatially weighted average concentration (SWAC) was calculated for these parameters using the natural neighbors approach. The approach for developing natural neighbors and its application to estimate sediment TOC and chemical concentrations in the surface sediment are described in the subsections that follow.

4.2.1 Natural Neighbors Approach

To calculate SWACs, natural neighbor interpolations were used. In this approach, a grid of values is produced, where each cell value is calculated by finding its Thiessen polygon relative to neighboring sample points, then taking the mean of those sample points weighted by the proportions of the sample Thiessen polygon areas intersected by the cell's polygon. Thus, the value of each grid cell is proportional to the average of the area of the original Thiessen polygon set covered by that cell's Thiessen polygon. A SWAC from a natural neighbor interpolation is the mean of the cell values within the Study Area, and has the same value as a SWAC from Thiessen polygons for the same area and data.

4.2.2 Total Organic Carbon in Sediment

Using the approach for creating natural neighbors described above in Section 4.2.1, a spatially weighted value for the percent of TOC in the sediment was obtained based on 1,329 sediment samples. For the model, a normal distribution was used with a mean concentration of 1.71% and a standard deviation of 0.028% (defined by the standard error of the empirical data).

4.2.3 Chemical Concentrations in Sediment

For each modeled chemical, a SWAC was calculated using the natural neighbors approach (Section 4.2.1). Table 4-3 presents the detection frequency and SWAC for each modeled chemical.

Table 4-3. Spatially Weighted Average Concentrations in Sediment

Chemical	Detection Frequency	Natural Neighbors SWAC (µg/kg dw)
PCBs		
PCB 17	246/253	1.07
PCB 77	254/266	0.185
PCB 118	40/96	3.28
PCB 126	251/266	0.0175
PCB 167	264/266	0.230
Total PCBs ^a	872/1,103	92.6
Dioxins and Furans		
2,3,4,7,8 PeCDF	173/219	0.0115
Pesticides		
4,4'-DDD	951/1,128	6.26
4,4'-DDE	928/1,125	3.43
4,4'-DDT	769/1,113	14.8
Aldrin	252/1,034	0.466
alpha-HCH	206/1,072	0.267
beta-HCH	443/1,083	1.28
Dieldrin	246/1,078	0.536
gamma-HCH	182/1,083	0.706
Heptachlor	72/1,083	0.216
Heptachlor epoxide	87/1,082	0.290
Sum DDD	969/1,128	8.89
Sum DDE	933/1,125	4.22
Sum DDT	856/1,127	17.3
Total chlordane	734/1,083	2.40
Total DDx	1,021/1,128	30.3

^a Total PCBs were calculated as the sum of congeners, when available. When congener data were not available, the sum of Aroclors was used.

DDD – dichlorodiphenyldichloroethane
DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
HCH – hexachlorocyclohexane

PCB – polychlorinated biphenyl
~~PeCDF – pentachlorodibenzofuran~~
SWAC – spatially weighted average concentration
total DDx – sum of all six DDT isomers (2,4'-DDD, 2,4'-DDE, 2,4'-DDT, 4,4'-DDD, 4,4'-DDE, and 4,4'-DDT)

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Distributions were not included for this parameter in calibration. Because the primary purpose of model development for this report was generation of preliminary remediation goals, the uncertainty surrounding estimates of sediment concentration was not a primary concern of model calibration. To develop PRGs there must be an assumed change in sediment chemical concentrations from current conditions. Therefore, it was necessary to define current conditions. The SWAC was assumed to represent current conditions, and uncertainties surrounding estimates of the SWAC would also apply to alternative conditions (such as the PRGs).

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5.0 BIOAVAILABLE FRACTION AND NON-SPECIES-SPECIFIC BIOLOGICAL PARAMETERS

Site-specific data for the bioavailable fractions and many general biological parameters in the Arnot and Gobas mechanistic model were not available. Thus, literature values were assigned to these parameters, and distributions were created when appropriate.

5.1 RESISTANCE TO CHEMICAL UPTAKE CONSTANTS

The value used in the model for uptake constant A (UA) was 6.0×10^{-5} and that used for uptake constant B (UB) was 5.50 (Gobas and Arnot 2005; Arnot and Gobas 2004). Based on comments from EPA on the mechanistic model developed as part of the Round 2 Report (EPA 2008a), these parameters were not calibrated, and thus no distribution was developed.

5.2 DIETARY CHEMICAL TRANSFER EFFICIENCY

Dietary chemical transfer efficiency (E_D) is described by K_{OW} and two dietary chemical transfer constants (EDA and EDB). Both EDA and EDB were taken from Arnot and Gobas (2004). The value used for constant EDA was 3×10^{-7} , and the value used for constant EDB was 2.0. No distributions were applied to these values because of a lack of information on parameter value uncertainty.

5.3 PROPORTIONALITY CONSTANTS

The value used for the non-lipid organic matter (NLOM)-octanol proportionality constant (BETA) was 0.035 (unitless) (Arnot and Gobas 2004). Based on comments from EPA on the mechanistic model developed as part of the Round 2 Report, these parameters were not calibrated, and thus no distribution was developed (EPA 2008a).

For the non-lipid organic carbon (NLOC)-octanol proportionality constant (GAMMA), a value of 0.350 (unitless) was obtained from Arnot and Gobas (2004). As in the Round 2 Report mechanistic model, no distribution was used for this parameter.

5.4 METABOLISM

Metabolism (K_M) was included only for those chemicals known to be metabolized. These included select PCB congeners (PCB 77 and PCB 126), dioxins (1,2,3,7,8-pentachlorodibenzo-*p*-dioxin [CDD] and 2,3,7,8-tetraCDD), furans (1,2,3,4,7,8-hexadibenzofuran [CDF], 2,3,4,7,8-pentaCDF, and 2,3,7,8-tetraCDF), and DDTs (4,4'-DDT and sum DDT). These chemicals include PCB 77, PCB 126, 2,3,4,7,8-PeCDF, 4,4'-DDT, and sum DDT. The application of metabolism rates on a chemical- and species-specific basis is discussed in detail in Section 6.6 of this Appendix for PCBs and DDTs and in Section 8.4 of this appendix for dioxins and furans.

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6.0 SPECIES-SPECIFIC BIOLOGICAL DATA

The trophic groups modeled, and the representative species for which LWG data are available (listed in parentheses), are as follows:

- Phytoplankton/algae
- Zooplankton
- Benthic invertebrate filter feeders (clams, *Corbicula fluminea*.)
- Benthic invertebrate consumers¹
- Epibenthic invertebrate consumers (crayfish, unidentified species)
- Foraging fish (sculpin, *Cottus* spp.)²
- Benthivorous fish (largescale sucker, *Catostomus macrocheilus*)³
- Omnivorous fish (common carp, *Cyprinus carpio*)
- Small piscivorous fish (smallmouth bass, *Micropterus dolomieu*)
- Large piscivorous fish (northern pikeminnow, *Ptychocheilus oregonensis*)

Site-specific data were available for clams, crayfish, sculpin, common carp, smallmouth bass, northern pikeminnow, and largescale suckers. Maps 6-1 to 6-7 provide information regarding the sample locations for these species. Circled locations indicate samples that were composited.

6.1 WEIGHTS, LIPID FRACTION, AND WATER CONTENT

Weight, lipid fraction, and water content data were derived from site-specific data for most organisms. These data were not available for phytoplankton/algae, zooplankton, and worms, so literature values were identified for these parameters.

6.1.1 Phytoplankton/Algae

Weight data for phytoplankton/algae were not required by the model. The lipid fraction and water content fraction values for phytoplankton/algae were calculated from Mackintosh et al. (2004). The values presented in this study are an aggregate of brown algae, green algae, and phytoplankton/algae collected from a tow net. A triangle distribution was assigned for the

¹ A generalized category designed to represent oligochaetes, insect larvae, and amphipods.

² This trophic group was also used to represent black crappie for PRG development.

³ This trophic group was also used to represent brown bullhead for PRG development.

lipid fraction with a nominal value of 0.00123 and minimum and maximum of 0.0008 and 0.002, respectively. The water content fraction was calculated by subtracting the reported NLOC fraction (nominal value of 0.0433 and minimum and maximum of 0.006 and 0.063, respectively) and lipid fractions from 1. This estimate of water content does not include consideration of constituents other than lipids, carbon, and moisture because they were not available. A triangle distribution was also assigned for water content fraction with a nominal value of 0.955 and a minimum and maximum of 0.935 and 0.993, respectively.

6.1.2 Zooplankton

The average weight of zooplankton was estimated from Giles and Cordell (1998). Assuming 90% moisture content, the nominal value value for zooplankton was 1.4×10^{-7} kg. A triangle distribution was assigned with the nominal value and the minimum and maximum of 3.3×10^{-8} and 2.3×10^{-7} , respectively, reflecting the range presented in Giles and Cordell (1998). The lipid fraction was calculated from Evjemo and Olsen (1997), again assuming a moisture content of 90%. A triangle distribution was assigned with the nominal value of 0.01 and a minimum and maximum of 0.009 and 0.011, respectively, reflecting the range from Evjemo and Olsen (1997). The moisture content fraction used for zooplankton was 0.9 (Kuroshima et al. 1987) [as cited in Delbare et al. (1996)]. A triangle distribution was assigned with a mean of 0.9 and a minimum and maximum of 0.80 and 0.98, respectively, as determined using best professional judgment.

6.1.3 Invertebrates

Site-specific data were available for benthic invertebrate filter feeders (clams) and epibenthic invertebrate consumers (crayfish). For these two taxa, distributions for weight, lipid fraction, and water content (Table 6-1) were assigned based on the criteria described in Section 2.0.

Table 6-1. Weight, Lipid Fraction, and Water Content for Invertebrate Species

Species	Parameter	Count ^a	Distribution Type	Nominal Value	SD or Min and Max ^b	Source
Benthic invertebrate filter feeders (clams)	Weight (kg)	2,223	Normal	0.00125	SD = 1.3×10^{-5}	BERA database
	Lipid fraction	42	Normal	0.022	SD = 0.0011	BERA database
	Water content fraction	38	Normal	0.86	SD = 0.0029	BERA database
Benthic invertebrate consumers	Weight (kg)	NA	Triangle	5.33×10^{-6}	min = 1.4×10^{-6} max = 6.0×10^{-6}	Kraaij et al. (2001); Millward et al. (2001); Bervoets et al. (2003)
	Lipid fraction	NA	Triangle	0.015	min = 0.008 max = 0.042	Weston et al. (2002); Kraaij et al. (2001); Lyytikainen et al. (2003); BERA database
	Water content fraction	NA	Triangle	0.80	min = 0.72 max = 0.88	best professional judgment

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Table 6-1. Weight, Lipid Fraction, and Water Content for Invertebrate Species

Species	Parameter	Count ^a	Distribution Type	Nominal Value	SD or Min and Max ^b	Source
Epibenthic invertebrate consumers (crayfish)	Weight (kg)	272	Normal	0.0435	SD = 0.00071	BERA database
	Lipid fraction	32	Normal	0.0078	SD = 0.00045	BERA database
	Water content fraction	32	Normal	0.74	SD = 0.0031	BERA database

^a Count represents the number of individuals for weight data and the number of composite samples for all other parameters.

^b The standard error of the data was used to describe the standard deviation of estimates of the mean.

BERA – baseline ecological risk assessment

NA – not applicable

SD – standard deviation

For benthic invertebrate consumers (worms, amphipods, midges, etc.), values were assigned based on literature and best professional judgment. Weight data for three detrital/deposit feeding species (*Chironomus riparius*, *Limnodrilus hoffmeisteri*, and *Corophium voluntator*) were examined (Kraaij et al. 2001; Millward et al. 2001; Bervoets et al. 2003) and used to define a triangle distribution. The lipid fraction for this trophic group was also evaluated using literature data on several different species (*Corphium* spp., *Nereis vexillosa*, and *Chironomus* spp.) (Weston et al. 2002; Kraaij et al. 2001; Lyytikäinen et al. 2003). In addition, information on lipid content collected prior to exposure for LWG bioaccumulation tests was considered. These studies used worm species found in the [LWR-Lower Willamette River](#) (*Lumbriculus* spp.) (Windward and Integral 2005). Table 6-1 summarizes distribution selections for weight, lipid content, and water content fraction for benthic invertebrate consumers.

6.1.4 Fish Species

Site-specific data were available for all modeled fish species, which included sculpin, largescale sucker, carp, smallmouth bass, and northern pikeminnow. Weight, lipid fraction, and water content fraction data were calculated using data from the project database. Before use, the data were examined to ensure that all samples were taken within the Study Area (RM 2 to RM 11). Table 6-2 presents the values and distributions that were used for the parameters for each species.

Table 6-2. Weight, Lipid Fraction, and Water Content for Fish Species

Species	Parameter	Count ^a	Distribution Type	Mean	Standard Deviation ^b
Sculpin	Weight (kg)	627	Normal	0.0196	0.00039
	Lipid fraction	38	Normal	0.041	0.0016
	Water content fraction	38	Normal	0.75	0.0023
Largescale sucker	Weight (kg)	34	Normal	0.794	0.012
	Lipid fraction	6	Normal	0.076	0.0052

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Table 6-2. Weight, Lipid Fraction, and Water Content for Fish Species

Species	Parameter	Count ^a	Distribution Type	Mean	Standard Deviation ^b
Carp	Water content fraction	6	Normal	0.71	0.0054
	Weight (kg)	75	Normal	2.48	0.066
	Lipid fraction	15	Normal	0.088	0.0053
Smallmouth bass	Water content fraction	15	Normal	0.69	0.0047
	Weight (kg)	228	Normal	0.395	0.18
	Lipid fraction	32	Normal	0.054	0.0021
Northern pikeminnow	Water content fraction	32	Normal	0.71	0.0033
	Weight (kg)	27	Normal	0.558	0.048
	Lipid fraction	6	Normal	0.053	0.008
	Water content fraction	6	Normal	0.719	0.0088

^a Count represents the number of individual fish for weight data and the number of composite samples for all other parameters.

^b The standard error of the data was used to describe the standard deviation of estimates of the mean.

6.2 DIETARY ABSORPTION EFFICIENCIES

Dietary absorption efficiencies of lipids, NLOM, and water were generally taken from Arnot and Gobas (2004) because site-specific data were not available for these parameters. Table 6-3 presents the values that were assigned to each of these parameters.

Table 6-3. Dietary Absorption Efficiency Fractions

Species	Species Included	Dietary Absorption Efficiency ^a	Nominal Value
Zooplankton	NA	Lipid (eL)	0.72
		NLOM (eN)	0.72
		Water (eW)	0.25
Invertebrates	Include benthic invertebrate filter feeders (clams), benthic invertebrate consumers, and epibenthic invertebrate consumers (crayfish)	Lipid (eL)	0.75
		NLOM (eN)	0.75
		Water (eW)	0.25
Fish species	Sculpin, largescale suckers, carp, smallmouth bass, and northern pikeminnow	Lipid (eL)	0.92
		NLOM (eN)	0.60
		Water (eW)	0.25

Source: Arnot and Gobas (2004)

^a Abbreviations for dietary absorption efficiencies used in the model are provided in parentheses for reference.

NA – not applicable

Based on comments from EPA on the mechanistic model developed as part of the Round 2 Report (EPA 2008a), no distributions were used for lipid and NLOM dietary absorption efficiencies. Additionally, no distribution was assigned to dietary absorption of water

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inasmuch as the model is not sensitive to this parameter because water is not a significant reservoir for hydrophobic organics compared to lipid and NLOM (Arnot and Gobas 2004). These parameters were not required for phytoplankton/algae, but all other modeled species are represented in the table.

6.3 POREWATER VENTILATION

The fraction of porewater ventilated by each species was determined by best professional judgment. In addition, porewater ventilation fractions were altered from the previous mechanistic model based on agency comments that suggested eliminating porewater ventilation for all fish except sculpin (EPA 2006). Table 6-4 presents the values used for each species in this model.

Table 6-4. Fraction of Porewater Ventilating

Species	Distribution Type	Nominal Value	Minimum and Maximum	Rationale
Phytoplankton/algae	Point estimate	0	NA	Live in water column and are not exposed to porewater.
Zooplankton	Point estimate	0	NA	Live in water column and are not exposed to porewater.
Benthic invertebrate filter feeders (clams)	Uniform	0.05	Min = 0.01 Max = 0.10	Live in the sediment and use short siphon to ventilate water from just above the sediment surface.
Benthic invertebrate detrital/deposit feeders)	Uniform	0.05	Min = 0.01 Max = 0.10	Primarily dwell beneath sediment.
Epibenthic invertebrate consumers (crayfish)	Uniform	0.05	min = 0.01 Max = 0.10	Crayfish live in burrows in the sediment and forage on the sediment.
Sculpin	Uniform	0.05	Min = 0.01 Max = 0.10	Some sediment surface feeding. Agency comments suggested eliminating FPW for all fish except sculpin (EPA 2006).
Largescale suckers	Point estimate	0	NA	Limited contact with sediment. Agency comments suggested eliminating FPW for all fish except sculpin (EPA 2006).
Carp	Point estimate	0	NA	Some bottom feeding, but primarily lives in water column. Agency comments suggested eliminating FPW for all fish except sculpin (EPA 2006).
Smallmouth bass	Point estimate	0	NA	Primarily swim and feed in water column.
Northern pikeminnow	Point estimate	0	NA	Primarily swim and feed in water column.

EPA – US Environmental Protection Agency

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FPW – fraction of porewater ventilated
NA – not applicable

6.4 GROWTH RATE CONSTANT

The growth rate for most modeled species is approximated by the model using an equation that is based on the weight parameter and is specialized for aquatic organisms. However, no weight data were required for phytoplankton/algae, so a growth rate constant was required. A triangular distribution was assigned with a nominal value of 0.08 per day, a minimum of 0.03 per day, and maximum of 0.13 per day (Arnot and Gobas 2004).

6.5 SCAVENGING EFFICIENCY (FILTER FEEDERS ONLY)

Scavenging efficiency is required for only benthic invertebrate filter feeders (clams). A value of 1.0 was derived from Morrison et al. (1996, as cited in Arnot and Gobas 2004), Reenders et al. (1989), and Ten Winkel and Davids (1982). No distribution was developed for this parameter.

6.6 CHEMICAL-SPECIFIC METABOLISM

Chemical-specific metabolism is one of the four chemical elimination routes in the Arnot and Gobas mechanistic model (Arnot and Gobas 2004).⁴ The metabolism, or biotransformation, of some chemicals explains why they are not bioaccumulated in the tissues of higher trophic level organisms to the extent that would be predicted. A review of literature regarding metabolic rate constants (K_{MS}) indicates that some members of the chemical classes being modeled for Portland Harbor are likely metabolized (e.g., Niimi 1996; Sijm et al. 1993; Opperhuizen and Sijm 1990; Konwick et al. 2006). While these and other sources indicate that metabolism is likely occurring, much uncertainty exists regarding the rates at which chemicals are metabolized.

6.6.1 PCBs

A study of chemical concentrations in fish tissue collected from the Willamette River examined the change in chemical compositions in black crappie, common carp, and smallmouth bass tissue over several years (Sethajintanin et al. 2004). The results of this study indicated that lower-chlorinated PCB congeners are metabolized to a greater extent by fish than are the higher-chlorinated congeners. Similar conclusions have been made from other studies (Niimi 1996).

⁴ The other three routes by which chemical concentrations in tissue may decrease are through respiratory (gill) elimination, fecal egestion, and growth dilution (Arnot and Gobas 2004).

6.6.2 Organochlorine Pesticides

Additionally, in their study of the Willamette River, Sethajintanin et al. (2004) also examined organochlorine pesticide concentrations in fish tissue, and found that 4,4'-DDD, 4,4'-DDE, and 4,4'-DDT are the most commonly detected chemicals in this class. Of these chemicals, 4,4'-DDE was determined to be the most persistent of these chemicals, while it was found that 4,4'-DDT was metabolized by fish, breaking down mostly into 4,4'-DDE (Konwick et al. 2006; Sethajintanin et al. 2004). Although Sethajintanin et al. (2004) did not evaluate the metabolism of dioxins and furans in fish in the Willamette River, other studies have confirmed that most dioxins and furans are metabolized to some degree (Sijm et al. 1993; Opperhuizen and Sijm 1990). Recent EPA guidance regarding the evaluation of dioxins and furans in risk assessments also asserts that dioxins and furans are metabolized by vertebrates (EPA 2008b).

In addition, although 4,4'-DDT is the most highly metabolized DDx isomer, it should be noted that DDD and DDE are also metabolized. DDT is the name that is commonly applied to 1,1,1-trichloro-2,2-bis(p-chlorophenyl)ethane. DDT has several isomeric forms, including o,p'-DDT (2,4'-DDT), but the collective ecological toxicity data on DDT has focused on p,p'-DDT (4,4'-DDT) as being the most toxicologically significant.

DDT and its primary metabolites, DDE and DDD, are persistent in the environment (USEPA 2007a) and can bioaccumulate. The degradation of 2,4'- and 4,4'-isomers of DDx is dependent upon environmental conditions, such as physicochemical properties of the soil (e.g., presence of molecular oxygen and organic carbon) and the microbial community structure. In the presence of oxygen, DDT can be transformed to DDE via dehydrohalogenation (Alvarez and Illman 2006). This degradation process can occur microbially or chemically and does not require an input of electrons. In addition, DDE can be further degraded to 4,4'-dichlorobenzophenone (DBP) and ultimately mineralized to carbon dioxide (Aislabie et al. 1999).

In anoxic environments, DDT is reductively dechlorinated by micro-organisms to DDD. This is a co-metabolic transformation because the degrading anaerobic microbes require an alternative carbon source, inasmuch as nutrients and energy cannot be derived exclusively from DDT (Aislabie et al. 1999). DDD can be further reductively dechlorinated and degraded to a variety of metabolites (Aislabie et al. 1999), including the following:

- DDMU – 1-chloro-2,2-bis(p-chlorophenyl)ethylene
- DDMS – 1-chloro-2,2-bis(p-chlorophenyl)ethane
- DDNU – 2,2-bis(p-chlorophenyl)ethylene
- DDOH – 2,2-bis(p-chlorophenyl)ethanol
- DDA – bis(p-chlorophenyl)-acetic acid
- DDM – bis(p-chlorophenyl)methane
- DBH – 4,4'-dichlorobenzhydrol

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- DBP – 4,4'-dichlorobenzophenone

Research indicates that DDT may be degraded by ligninolytic fungi in the presence of oxygen (Aislabie et al. 1999). In fact, DDx may be completely mineralized to carbon dioxide by several groups of fungi (Bennet et al. 2002). DDT can be photolytically transformed to DDE in the presence of sunlight and further degraded photolytically to DBP and DDMU, although this process is less important than microbial biotransformation.

The literature suggests that DDT can also be metabolized to DDE in higher trophic levels (e.g., squid, fish, and mammals) (Tanabe et al. 1994; Nortstrom 2002). A group of oxygenases (CYP450) in vertebrates can rapidly transform 4,4'-DDT to 4,4'-DDE (Nortstrom 2002). Nortstrom also reported that 2,4'-DDT may be less persistent than the 4,4'-isomer because it can be degraded to water-soluble metabolites and subsequently excreted.

6.6.3 Selection of Metabolic Rates

Table 6-5 presents a summary of the chemicals selected for modeling in the Portland Harbor mechanistic model and provides information regarding the extent to which these chemicals are expected to be metabolized.

Table 6-5. Summary of the Metabolism of Modeled Chemicals by Fish

Chemical	Significant Metabolism?	Rationale	References
PCBs			
PCB 118	No	One of the most abundant of PCB congeners in fish tissue from LWR-Lower Willamette River samples (Sethajintanin et al. study), indicating that it is relatively persistent in the environment.	Niimi (1996); EPA (2008b); Sethajintanin et al. (2004)
PCB 77 and PCB 126	Yes	Low concentrations of PCB 77 and PCB 126 in Willamette River tissue, moderate chlorination, so likely to be metabolized by fish.	
Total PCBs	No	Individual congeners are known to be metabolized, but those congeners that make up the majority of the total PCB sum are not highly metabolized.	
Dioxins and Furans			
2,3,4,7,8-PeCDF	Yes	Dioxins and furans are known to be metabolized by vertebrates, especially those with lower chlorine contents (e.g. 4 to 6 chlorines).	Niimi (1996); EPA (2008b)

Table 6-5. Summary of the Metabolism of Modeled Chemicals by Fish

Chemical	Significant Metabolism?	Rationale	References
DDTs			
2,4'-DDx isomers	No	Not highly metabolized by fish	Konwick et al. (2006);
4,4'-DDD and 4,4'-DDE	No	Little metabolism has been observed for DDDs or DDEs. Because DDEs are the major breakdown product of DDTs and because they are not highly metabolized, DDEs were found in fish tissue samples from the LWR <u>Lower Willamette River</u>	Sethajintanin et al. (2004)
4,4'-DDT	Yes	Metabolism of DDTs by fish has been reported in various studies at significant rates.	

DDD – dichlorodiphenyldichloroethane

DDE – dichlorodiphenyldichloroethylene

DDT – dichlorodiphenyltrichloroethane

PCB – polychlorinated biphenyl

~~PeCDF~~ – ~~pentachlorodibenzofuran~~

total DDx – sum of all six DDT isomers (2,4'-DDD, 2,4'-DDE, 2,4'-DDT, 4,4'-DDD, 4,4'-DDE, and 4,4'-DDT)

To evaluate options regarding the treatment of ~~K_M metabolic rate constants~~ and their calibration, models developed for other aquatic systems were examined. In a Lake Ontario food web model study (Morrison et al. 1999), the model was developed to predict concentrations of dioxins/furans and PCB congeners in the tissues of aquatic organisms. Chemicals that were known to metabolize were calibrated and then the metabolic rate was determined by attempting to minimize the difference between the predicted and empirical tissue concentrations (for four fish species and for crustaceans). The selected values were compared to literature studies, and it was concluded that these values were generally in the range of realistic metabolic rates for the dioxin/furan and PCB congeners that were modeled.

Another mechanistic model study was developed for an aquatic food web in Venice Lagoon, Italy (Micheletti et al. 2008). As with the Lake Ontario model, this model was developed for dioxins/furans and dioxin-like PCBs. Non-metabolizing chemicals were calibrated first, and then chemicals known to be metabolized were calibrated, attempting to minimize the difference between model-predicted and empirical tissue concentrations for both invertebrates and fish. It was assumed that the maximum acceptable K_M value was 0.5/day. The model was calibrated using data from three exposure areas, and the selected K_M values (and other calibrated parameter values) were then verified using data from three additional exposure areas.

For the Portland Harbor mechanistic model, nominal values and distributions for K_M values were developed for the chemicals identified in Table 6-5 as being metabolized to a significant extent. Metabolic rates were initially applied only to fish, based on research indicating that vertebrates metabolize chemicals at a higher rate than invertebrates (EPA 2008b). However, based on the available data, metabolic rates were applied to invertebrates

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when applicable. In a recently published study, Arnot et al. (2008) developed a database of fish biotransformation rates that were calculated for a wide variety of chemicals based on bioconcentration factor (BCF), total elimination rate (K_T), and chemical half-lives published in other papers. Table 6-6 presents a summary of the ~~K_M metabolic rate constant~~ data available in the Arnot et al. (2008) database for chemicals identified as significantly metabolized in Table 6-5. A nominal K_M value was calculated as equal to the average of the values presented by Arnot et al. (2008). Because these values are highly uncertain, K_M was calibrated to improve model predictions of empirical data. For model calibration, a uniform distribution was assigned equal to a range of a minimum of 0 to a maximum equal to 1 order of magnitude greater than the nominal value.

Table 6-6. Selection of Metabolic Rate Constants (1/day) for Metabolized Chemicals

Chemical	Summary of Arnot et al. (2008) K_M Values				Selected K_M Values	
	Average	Count	SD	Database Range	Nominal Value	Distribution ^a
PCBs						
PCB 77	0.03	2	0.01	0.02 – 0.04	0.03	0 – 0.3
PCB 126	0.003	1	NA	0.003	0.003	0 – 0.03
Dioxins and Furans						
2,3,4,7,8-PeCDF	0.03	1	NA	0.03	0.03	0 – 0.3
DDTs						
4,4'-DDT	0.01	4	0.02	0.0003 – 0.03	0.01	0 – 0.1
Sum DDT ^c	NA	NA	NA	NA	0.005 ^b	0 – 0.05 ^b

Source: Arnot et al. (2008)

^a The lower bound of the uniform distribution was set equal to 0. The upper bound was set equal to the lower of either 0.5/day or to 1 order of magnitude greater than the nominal value.

^b As a conservative estimate, the metabolic rate for sum DDT was estimated as equal to one-half of the metabolic rate selected for 4,4'-DDT, although 4,4'-DDT made up more than 50% of sum DDT.

^c Sum DDT is the sum of 2,2'- DDT and 4,4'-DDT. The former is not expected to metabolize significantly.

DDT – dichlorodiphenyltrichloroethane

NA – not applicable

~~PeCDF – pentachlorodibenzofuran~~

K_M – metabolic rate constant

PCB – polychlorinated biphenyl

SD – standard deviation

The general process of model calibration is as follows and as described in Section 5.2.5.3 and Figure 5-1 (of the Bioaccumulation Modeling Report). Non-chemical-specific parameters were calibrated first for all chemicals (using a non-metabolized chemical). Chemical-specific parameters (K_{OW} and chemical concentration in water) were calibrated second. Lastly, for metabolized chemicals, the K_M value was calibrated using the ranges and nominal values described here. It should also be noted that the nominal value of the K_M was used in the model during the calibration of the K_{OW} and chemical concentration in water for metabolized chemicals.

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6.7 DIETARY ASSUMPTIONS

The diets of each modeled species were developed by conducting literature reviews, interviewing fish biologists, and reviewing agency comments (EPA 2006, 2008a) in order to best reflect the diets of each species. However, because of the limited number of species that were modeled, dietary consumption described in the literature of species (i.e., prey) not included in the model had to be reassigned to other species using best professional judgment. The species included in the current model were based on discussions with and comments from the EPA and its partners (EPA 2006), and this list is the same as the one in the Round 2 Report mechanistic model (Integral et al. 2007). Thus, most diets are necessarily simplified. For example, sculpin are known to eat juvenile fish, but this category was not included in this version of the mechanistic model. For other fish species, sculpin were used to represent juvenile fish. Because cannibalism and eating fish designated as higher up in the food web are not possible in the model, sculpin cannibalism and sculpin consumption of juvenile fish were represented by the consumption categories of benthic invertebrate consumer and benthic invertebrate filter feeder. These surrogate selections were based primarily on a consideration of life history and lipid content in the previously modeled juvenile fish (Windward 2005) and the three invertebrates.

Table 6-7 presents the diet percentages used to define the uniform distributions for model calibration and provides the rationales for these diets.

Table 6-7. Diets for Modeled Species

Prey Item	Distribution Type	Nominal Value (%)	Range ^a (%)	Rationale and Source
Zooplankton Diet				
Phytoplankton/algae	Point estimate	100	NA	Using best professional judgment, it was assumed that the portion of carnivorous zooplankton in the LWR <u>Lower Willamette River</u> is insignificant as compared to planktivores.
Benthic Invertebrate Filter Feeder (BIF) Diet based on Clams				
Sediment solids	Uniform	70	50 – 80	Diet was based on Pechenick (1991), Kraaij et al. (2001), and Zaranko et al. (1997).
Phytoplankton/algae	Uniform	30	20 – 50	
Benthic Invertebrate Consumer (BIC) Diet based on Worms, Amphipods, Insect Larvae, etc.				
Sediment solids	Uniform	95	85 – 100	Diet was developed based on a combination of insect larvae, oligochaete, and amphipod diets from the previous model (Windward 2005), as well as Pechenick (1991) and Zaranko et al. (1997).
Phytoplankton/algae	Uniform	5	0– 15	
Epibenthic Invertebrate Consumer (EIC) Diet based on Crayfish				
Sediment solids	Uniform	2	0 – 4	Crayfish diets and distributions are highly uncertain because they are thought to feed non-selectively. Best professional judgment was used to resolve these
Phytoplankton/algae	Uniform	10	0 – 20	

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Table 6-7. Diets for Modeled Species

Prey Item	Distribution Type	Nominal Value (%)	Range ^a (%)	Rationale and Source
Zooplankton	Uniform	10	0 – 20	differences in available studies (Pechenik 1991; Evans-White et al. 2001).
BIF (clams)	Uniform	18	0 – 35	
BIC	Uniform	60	25 – 75	
Sculpin Diet				
Sediment solids	Uniform	0	0 – 5	Fish consumption, cannibalism, and worm consumption likely occupy the highest percentages of sculpin diets. The fish consumption portion of the diet was transferred to clams, worms, and crayfish. Studies do not indicate specific consumption of sediment (although sculpin likely ingest some), zooplankton, clams, or crayfish. Sources included Northcote (1954) and Brown et al. (1995).
Zooplankton	Uniform	0	0 – 5	
BIF (clams)	Uniform	15	0 – 50	
BIC	Uniform	80	25 – 90	
EIC (crayfish)	Uniform	5	0 – 10	
Largescale Sucker Diet				
Sediment solids	Uniform	5	1 – 15	Personal communication with Charles Lee (2006) indicated that sucker diet consisted of 50% clams and 50% worms. Best professional judgment was used to reconcile differences between the information provided above and information from Jorgensen (1979) and stomach content analysis (Integral et al. 2004)
Phytoplankton/algae	Uniform	25	0 – 60	
Zooplankton	Uniform	15	5 – 25	
BIF (clams)	Uniform	10	5 – 15	
BIC	Uniform	25	15 – 35	
EIC (crayfish)	Uniform	20	0 – 40	
Carp Diet				
Sediment solids	Uniform	5	0 – 10	The carp diet was based on the diet used in the previous model (Windward 2005) from studies conducted in the Hanford Reach of the Mid-Columbia River. Best professional judgment was used to resolve differences between Gray and Daubble (2001) and Fishbase (2004).
Phytoplankton/algae	Uniform	45	30 – 60	
BIF (clams)	Uniform	10	5 – 15	
BIC	Uniform	40	25 – 55	
Smallmouth Bass Diet				
Sediment solids	Point estimate	0	NA	Based on the diet used in the previous model, but replaced peamouth and juvenile fish consumption with sculpin. Best professional judgment was used to resolve difference between ODFW (2005), Zimmerman (1999), and LWR-Lower Willamette River gut content survey (Integral et al. 2004)
BIC	Uniform	5	0 – 30	
EIC (crayfish)	Uniform	5	0 – 30	
Sculpin	Uniform	90	50 – 100	
Northern Pikeminnow Diet				
Sediment solids	Point estimate	0	NA	ODFW study conducted in the LWR-Lower Willamette River indicated that juvenile salmon were a major part of the pikeminnow diet (2005). All fish consumption (juvenile fish, juvenile chinook, peamouth, and sculpin) was combined under the sculpin prey category. Best professional judgment was
Phytoplankton/algae	Uniform	4	0 – 10	
BIF (clams)	Uniform	5	0 – 10	
BIC	Uniform	26	15– 45	

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Table 6-7. Diets for Modeled Species

Prey Item	Distribution Type	Nominal		Rationale and Source
		Value (%)	Range ^a (%)	
EIC (crayfish)	Uniform	40	25 – 65	used to resolve difference between the ODFW (2005), Gray and Daubble (2001), Buchanan et al. (1981), and Zimmerman (1999).
Sculpin	Uniform	25	0 – 60	

^a Uniform distributions were used for all dietary parameters in model calibration.

NA – not applicable

BIC – benthic invertebrate consumer

BIF – benthic invertebrate filter feeder

EIC – epibenthic invertebrate consumer

~~LWR – Lower Willamette River~~

ODFW – Oregon Department of Fish and Wildlife

Sediment and tissue consumption was determined as a percentage of the species' overall diet. The model is set up to normalize these dietary fractions to ensure that they always equal 100% (see Appendix E for information regarding the design of the mechanistic model). For example, if all of the maximum values were selected for a given species, that species would be consuming greater than 100% of their diet. Thus, the relative proportions of the selected dietary parameters for each model run are used to calculate normalized dietary fractions that together add up to 100%. Model results in which normalized diets containing values for consumption that were below the minimums or in excess of maximums specified in Table 6-5 were rejected.

7.0 COMPARISON OF KEY MODEL PARAMETERS

This section presents a comparison of key model parameter values between the updated and the Round 2 Report mechanistic model (Table 7-1). The key parameters were identified by the sensitivity analysis performed as part of the Round 2 Report, and include the log K_{OW}, the chemical concentration in sediment and water, the mean water temperature, and the benthic invertebrate consumer lipid fraction.

Table 7-1. Comparison of Updated and Round 2 Report Mechanistic Model Key Parameter Values

Chemical	Updated Model			Round 2 Report Model		
	Distribution Type	Distribution Values	Calibrated Value	Distribution Type	Distribution Values	Calibrated Value
Concentration in Sediment Solids (µg/kg dw)						
Total PCBs		92.6 ^a	NA		72.1 ^a	NA
4,4'-DDD		6.26	NA		7.87	NA
4,4'-DDT		14.8	NA		15.3	NA
Sum DDD	Point estimate	8.89	NA	Point estimate	10.6	NA
Sum DDE		4.22	NA		4.63	NA
Sum DDT		17.3	NA		17.4	NA
Total DDx		30.3	NA		32.6	NA
Concentration in Water (filtered water) (ng/L)						
Total PCBs		0.217 (SE = 0.0244)	0.228		0.195 (SE = 0.0279)	0.189
4,4'-DDD		0.049 (SE = 0.0090)	0.053		0.0344 (SE = 0.00869)	0.0512
4,4'-DDT		0.017 (SE = 0.0021)	0.015		0.00496 (SE = 0.000895)	0.00441
Sum DDD	Normal	0.070 (SE = 0.013)	0.094	Normal	0.0502 (SE = 0.0124)	0.0744
Sum DDE		0.032 (SE = 0.0029)	0.038		0.0206 (SE = 0.00332)	0.0288
Sum DDT		0.022 (SE = 0.0024)	0.0217		0.00718 (SE = 0.00134)	0.00748
Total DDx		0.13 (SE = 0.017)	0.139		0.0779 (SE = 0.0161)	0.0493

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Table 7-1. Comparison of Updated and Round 2 Report Mechanistic Model Key Parameter Values

Chemical	Updated Model			Round 2 Report Model		
	Distribution Type	Distribution Values	Calibrated Value	Distribution Type	Distribution Values	Calibrated Value
Log Kow						
Total PCBs		7.40 (6.09 – 7.84)	6.14		6.67 (SE = 0.0667)	6.46
4,4'-DDD		6.05 (4.82 – 6.33)	5.83		6.02 (SE = 0.0602)	5.87
4,4'-DDT		6.72 (3.98 – 8.31)	6.31		6.91 (SE = 0.0691)	7.15
Sum DDD	Uniform	6.00 (4.80 – 6.31)	5.73	Normal	5.99 (SE = 0.0599)	5.79
Sum DDE		6.80 (4.22 – 6.87)	6.45		6.48 (SE = 0.0648)	6.61
Sum DDT		6.58 (3.98 – 8.19)	6.00		6.87 (SE = 0.0687)	6.64
Total DDx		6.65 (4.34 – 7.08)	5.91		6.47 (SE = 0.0647)	6.28
Non-Chemical-Specific Parameters						
Water temperature	Normal	13.9 (SE = 1.7)	13.7	Normal	13.56 (SE = 1.60)	14.99
BIC lipid content	Triangle	0.015 (0.008 – 0.042)	0.014	Triangle	0.015 (0.008 – 0.042)	0.017

^a The sediment SWAC for total PCBs was calculated using only Aroclor data for the Round 2 Report mechanistic model. For the updated model, a hybrid version of total PCBs was used in which congener data was used when available, and Aroclor data was used at all remaining locations.

BIC – benthic invertebrate consumer

DDD – dichlorodiphenyldichloroethane

DDE – dichlorodiphenyldichloroethylene

DDT – dichlorodiphenyltrichloroethane

NA – not applicable

PCB – polychlorinated biphenyl

total DDx – sum of all six DDT isomers (2,4'-DDD, 2,4'-DDE, 2,4'-DDT, 4,4'-DDD, 4,4'-DDE, and 4,4'-DDT)

8.0 PARAMETERIZATION FOR DIOXIN AND FURAN CONGENER MODELING

This section presents the chemical-specific parameters needed to develop models for the dioxin and furan congeners. In general, the approaches used to parameterize these models follow those used for the other modeled chemicals.

8.1 CHEMICAL DATA

As discussed in Section 3.0 of this appendix, two chemical-specific parameters were required for the for the bioaccumulation model: the K_{ow} and the Henry's Law constant. Because the Henry's Law constant cancels itself out in the model calculations, no values were entered for this parameter. The sources and hierarchy for the sources used to develop chemical-specific K_{ow} values for the dioxin and furan congeners were the same as those used for other chemicals.

As for the other modeled chemicals, the best-estimate literature value was selected from EPA's ESB guidance documents when available or from the SPARC database. A uniform distribution was used for the K_{ow} when calibrating the mechanistic model, with the distribution range equal to the minimum and maximum values from the above literature sources. Table 8-1 shows the K_{ow} values used in the mechanistic model.

Table 8-1. K_{ow} Values for Dioxins and Furans (NEW)

Analyte	Literature log K_{ow} Values		
	Primary	Minimum	Maximum
Dioxins			
1,2,3,7,8-PentaCDD	7.06	6.49	7.56
2,3,7,8-TetraCDD	6.38	5.38	8.93
Furans			
1,2,3,4,7,8-HexaCDF	7.66	6.9	7.92
2,3,4,7,8-PentaCDF	6.95	6.56	7.82
2,3,7,8-TetraCDF	6.30	5.82	7.70

CDD – chlorodibenzo-*p*-dioxin

CDF – chlorodibenzofuran

K_{ow} – octanol-water partition coefficient

8.2 CHEMICAL CONCENTRATION IN SURFACE WATER

As described in Section 4.1.2 of this appendix, chemical concentrations in the water column for use in the mechanistic model were calculated using XAD water column samples collected during the seven sampling events at the five transect locations. The same weighted average approach that was used to calculate the Study Area-wide water averages was used for dioxins and furans, except that for non-detected values, one-half of the detection limit (DL) was used

to represent the non-detected values (rather than excluding these from the datasets). This change was made for dioxins and furans because of the generally lower detection frequencies for these chemicals as compared with those of other modeled chemicals. In addition, an alternate weighted average water concentration was calculated to further evaluate the impact of the low detection frequencies. In this approach (Option 2), if no detected values were available in a given step, the lowest half DL was used as the average for that step. In addition, the samples collected during a storm event⁵ were excluded in order to evaluate the potential impact of these samples on the estimated overall average water concentration (this was important for sensitivity analysis because the appropriate weight for the storm event was uncertain). This option was used considered for those congeners with detection frequencies of less than 50%. Table 8-2 presents the average and standard error surface water concentrations for the high- and low-flow values, along with the values used in the model to define the normal distribution. This table shows both Option 1 and Option 2 concentrations.

Table 8-2. Chemical Concentrations in Surface Water for Dioxins and Furans (NEW)

Analyte	DF	Surface Water Concentrations (ng/L) ^a					
		High Flow		Low Flow		Model Values	
		Mean	SE	Mean	SE	Mean	SE
Option 1 Concentrations							
Dioxins							
1,2,3,7,8-PentaCDD	9/26	3.4×10 ⁻⁶	1.2×10 ⁻⁶	4.6×10 ⁻⁶	3.4×10 ⁻⁶	4.3×10 ⁻⁶	2.9×10 ⁻⁶
2,3,7,8-TetraCDD	1/26	1.7×10 ⁻⁶	4.5×10 ⁻⁸	2.9×10 ⁻⁶	1.5×10 ⁻⁶	2.7×10 ⁻⁶	1.2×10 ⁻⁶
Furans							
1,2,3,4,7,8-HexaCDF	7/26	7.5×10 ⁻⁶	3.5×10 ⁻⁸	5.4×10 ⁻⁶	2.1×10 ⁻⁶	5.9×10 ⁻⁶	1.7×10 ⁻⁶
2,3,4,7,8-PentaCDF	7/26	3.3×10 ⁻⁶	4.9×10 ⁻⁷	3.6×10 ⁻⁶	1.4×10 ⁻⁶	3.5×10 ⁻⁶	1.2×10 ⁻⁶
2,3,7,8-TetraCDF	15/26	2.2×10 ⁻⁶	2.5×10 ⁻⁸	6.4×10 ⁻⁶	1.5×10 ⁻⁶	5.5×10 ⁻⁶	1.2×10 ⁻⁶
Option 2 Concentrations ^b							
Dioxins							
1,2,3,7,8-PentaCDD	9/26	3.0×10 ⁻⁶	1.5×10 ⁻⁶	1.1×10 ⁻⁶	2.3×10 ⁻⁷	1.5×10 ⁻⁶	5.1×10 ⁻⁷
2,3,7,8-TetraCDD	1/26	1.5×10 ⁻⁶	0	6.5×10 ⁻⁷	3.0×10 ⁻⁷	8.3×10 ⁻⁷	2.4×10 ⁻⁷
Furans							
1,2,3,4,7,8-HexaCDF	7/26	6.1×10 ⁻⁶	1.4×10 ⁻⁶	2.9×10 ⁻⁶	1.1×10 ⁻⁶	3.6×10 ⁻⁶	1.2×10 ⁻⁶
2,3,4,7,8-PentaCDF	7/26	3.3×10 ⁻⁶	4.9×10 ⁻⁷	2.1×10 ⁻⁶	9.6×10 ⁻⁷	2.4×10 ⁻⁶	8.6×10 ⁻⁷

^a When calculating mean and SE values, only non-detects were assumed to be equal to one-half of the DL.

^b Alternate water concentrations (Option 2) were calculated only for dioxin and furan congeners with detection frequencies of less than 50%.

CDD – chlorodibenzo-*p*-dioxin

⁵ Of the seven events during which water samples were collected, one of these was considered a storm event. See Section 4.1.2 of this appendix for details regarding the water data.

CDF – chlorodibenzofuran
DF – detection frequency
DL – detection limit
SE – standard error

8.3 CHEMICAL CONCENTRATION IN SEDIMENT

As discussed in Section 4.2.3 of this appendix, a SWAC was calculated for each modeled chemical using the natural neighbors approach (described in Section 4.2.1). Table 8-3 presents the detection frequency and SWAC for each modeled dioxin and furan. As with the other chemicals, distributions were not included for this parameter in calibration (see Section 4.2.3 of this appendix).

Table 8-3. Spatially Weighted Average Concentrations in Sediment (NEW)

Chemical	Detection Frequency	Natural Neighbors SWAC (µg/kg dw)
Dioxins		
1,2,3,7,8-PentaCDD	128/219	0.00025
2,3,7,8-TetraCDD	41/219	0.00010
Furans		
1,2,3,4,7,8-HexaCDF	197/219	0.00271
2,3,4,7,8-PentaCDF	173/219	0.0115
2,3,7,8-TetraCDF	145/219	0.0168

CDD – chlorodibenzo-*p*-dioxin

CDF – chlorodibenzofuran

dw – dry weight

SWAC – spatially weighted average concentration

8.4 CHEMICAL-SPECIFIC METABOLISM

This section presents a discussion of the development of chemical-specific K_{MS} for the dioxin and furan congeners, including evidence from the literature of the metabolism of these chemicals and a discussion of the relative metabolic rates across the dioxins and furan congeners.

8.4.1 Evidence of the Metabolism of Dioxins and Furans

Dioxins and furans, especially those with a lower number of chlorines (e.g., 4 to 6 chlorines), are widely known to be metabolized by vertebrates (Niimi 1996; EPA 2008b). Specifically for fish, the inclusion of calculated metabolic rates in the database prepared by Arnot et al. (2008) provides further support that fish can metabolize the various dioxin and furan congeners.

Support for the metabolism of dioxins and furans by invertebrates can be found in work performed for the Contaminant Assessment and Reduction Project (CARP) for the New

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York/New Jersey Harbor estuary (HydroQual 2007) and in a study that measured the uptake and elimination of a dioxin compound for invertebrates (Zhang et al. 2011):

- The HydroQual (2007) report found that calculated biota-sediment accumulation factors (BSAFs) for dioxin/furan congeners for clams, crabs, and worms were approximately 10 times lower than those for PCBs (for chemicals with similar K_{OW} s) and noted that “this suggests that either there is an inefficient transfer of dioxin/furan congeners from sediment, or that worms also possess the capacity to metabolize dioxin and furan congeners.”
- The Zhang et al. (2011) study, which used radiotracers to measure the uptake, assimilation efficiency, and elimination of 1,2,3,4,7,8- hexaCDD⁶ in marine phytoplankton, copepods, and fish, noted that the half-life of this dioxin of 2 to 25 days for copepods was lower than that observed for fish in other studies. According to Zhang et al. (2011), the results suggested that these invertebrates have a rapid metabolic biotransformation rate due to their small size and may indicate that copepods have an efficient elimination system for removing or metabolizing 1,2,3,4,7,8-hexaCDD.

When considering K_M data, it is important to recognize that other processes that influence chemical concentrations in tissue are likely to affect these data. For the purpose of the model, it is not necessarily important to make a distinction between metabolism and reduced uptake of a given chemical because both processes have the same outcome: a lower concentration of the chemical in tissue. Rather than attempting to capture all of the processes that exist, the goal of the bioaccumulation model is to replicate the system to the extent necessary to accurately predict tissue concentrations. Thus, the use of the K_M parameter as a surrogate for a combination of metabolism and reduced uptake is appropriate for the purpose of this model.

8.4.2 Relative Metabolic Rates Across Dioxin and Furan Congeners

In a study of the uptake and elimination of dioxins and furans by guppy, Loonen et al. (1994) found that the elimination rate constants of fish for dioxins were lower than those for furans. Although elimination rate constants are influenced by factors other than metabolism, this provides an indication of the pattern that might be expected in the metabolic rate data. Based on a review of the biotransformation rate data presented in the database developed by Arnot et al. (2008), the pattern noted by Loonen et al. (1994) appears to be relevant for K_M values. In addition, tissue-to-sediment ratios (equal to the average tissue concentration divided by the sediment SWAC) for the Lower Willamette River were calculated and compared for each of the modeled dioxin and furan congeners (Table 8-4). As can be seen in this table, the ratios

⁶ Zhang et al. (2011) did not identify the specific dioxin compound that was evaluated in this study. In a personal communication, the authors (Wang 2014) clarified that the compound used in their study was 1,2,3,4,7,8-hexachlorodibenzo-*p*-dioxin.

for the dioxins are higher than those for the furans, further supporting the idea that dioxins have lower metabolic rates as compared with the furans.

Table 8-4. Tissue-to-Sediment Ratios for Invertebrates and Fish (NEW)

Chemical	Tissue-to-Sediment Ratios ^a								
	Invertebrates			Fish					
	Clam	Cray-fish	Average	Sculpin	Carp	Small-mouth Bass	Black Crappie	Brown Bullhead	Average
Dioxins									
1,2,3,7,8-PentaCDD	0.84	0.80	0.82	2.0	5.4	5.4	1.9	2.5	3.5
2,3,7,8-TetraCDD	1.8	1.4	1.6	2.6	7.1	6.4	3.3	3.6	4.6
Furans									
1,2,3,4,7,8-HexaCDF	0.19	0.72	0.45	1.6	0.72	0.63	0.06	0.14	0.63
2,3,4,7,8-PentaCDF	0.07	0.15	0.11	0.18	0.21	0.48	0.02	0.07	0.19
2,3,7,8-TetraCDF	0.15	0.38	0.26	0.52	0.17	0.38	0.08	0.03	0.24

^a Ratios were calculated as the average empirical tissue concentration divided by the sediment SWAC.

CDD – chlorodibenzo-*p*-dioxin

CDF – chlorodibenzofuran

8.4.3 Development of Distributions

Because the modeled dioxins and furans were thought to be significantly metabolized, distributions were developed for these chemicals. As with the other chemicals, distributions were developed based on the available K_M data presented by Arnot et al. (2008), in which fish biotransformation rates were calculated for a wide variety of chemicals based on BCFs, total elimination rates (K_{TS}), and chemical half-lives published in other papers. Table 8-5 presents a summary of the K_M data available in the Arnot et al. (2008) database for dioxins and furans. A nominal K_M value was calculated as equal to the average of the values presented by Arnot et al. (2008). Because these values are highly uncertain, K_M was calibrated to improve model predictions of empirical data. For model calibration, a uniform distribution was assigned for each dioxin and furan. The bounds of the uniform distribution were set equal to the database range when chemical-specific data were available. For 1,2,3,4,7,8-hexaCDF, no chemical-specific data were provided in the database, and thus other hexa-furans were used as surrogate chemicals.⁷ In this case, a broader distribution was used based on the higher level of uncertainty associated with the K_M value for this chemical.

⁷ Loonen et al. (1994) found that there were differences in the uptake and elimination of the laterally substituted congeners (i.e., the 2,3,7,8-substituted congeners) as compared with the non-laterally substituted congeners (i.e., the non-2,3,7,8-substituted congeners). All of the modeled congeners detailed in this report were 2,3,7,8-substituted congeners, and thus only these congeners were considered as surrogates.

Table 8-5. Selection of Metabolic Rate Constants (1/day) for Metabolized Chemicals (NEW)

Chemical	Summary of Arnot et al. (2008) K _M Values				Selected K _M Values	
	Average	Count	SD	Database Range ^a	Nominal Value	Distribution
Dioxins						
1,2,3,7,8-PentaCDD	0.019	1	NA	0.005 – 0.07	0.019	0.005 – 0.07
2,3,7,8-TetraCDD	0.013	7	0.007	0.002 – 0.08	0.013	0.002 – 0.08
Furans						
1,2,3,4,7,8-HexaCDF ^b	0.06	2	0.01	0.02 – 0.2	0.06	0 – 0.6
2,3,4,7,8-PentaCDF	0.03	1	NA	0.009 – 0.1	0.03	0.009 – 0.1
2,3,7,8-TetraCDF	0.1	2	0.1	0.01 – 0.5	0.1	0.01 – 0.5

^a The database range is equal to the estimated 2.5th to 97.5th percentile from the database (Arnot et al. 2008).

^b No data were available in Arnot et al. (2008) for 1,2,3,4,7,8-hexaCDF. Thus, the two other 2,3,7,8-substituted hexa-furans (i.e., 1,2,3,6,7,8-hexaCDF and 2,3,4,6,7,8-hexaCDF) were used as surrogates for the development of the K_M distribution. Because of the uncertainty introduced with this approach, a broader distribution range (equal to zero to one order of magnitude above the average value) was used for this chemical.

CDD – chlorodibenzo-*p*-dioxin

CDF – chlorodibenzofuran

K_M – metabolic rate constant

NA – not applicable (insufficient data to calculate an SD)

SD – standard deviation

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MAPS

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